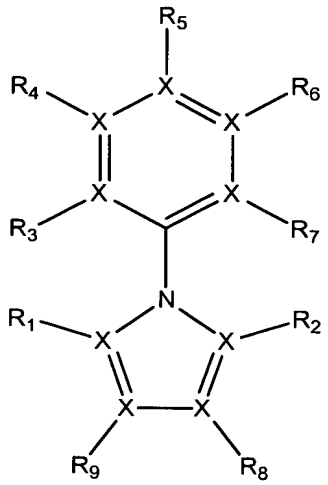
What is claimed is:

1. A compound of molecular weight from 200 to 1200 Daltons, and logP of -2.0 to +5.5, capable of interacting with the hydrophobic cavity and blocking the formulation of the fusion-active gp41 coiled core domain.

2. The compound of claim 1, which is negatively charged.

3. A compound having the following formula:



I

Wherein at least one of R_1, R_2 R_3, R_4, R_5, R_6, R_7, R_8, and R_9 contains COOH or other acidic groups.

4. The compound of claim 3, wherein X can be C or N; when C or N is at any X position, the corresponding R group may or may not be there.

5. The compound of claim 3, wherein X is either O or S; when X is either O or S, the bond with the next atom, such as C, will be a single bond and O or S will be unsubstituted.

6. A compound having formula I, wherein X is a carbon or its pharmaceutically acceptable salts,

Wherein:

R_1 and R_2 are independently selected from the group consisting of H, alkyl, alkenyl, alkynyl, halogen, CN, nitro, OH and OR, where R is alkyl;

R_3, R_4, R_5, R_6, R_7, R_8, and R_9 are each independently selected from the group consisting of H, alkyl, cycloalkyl, alkenyl, alkynyl, aryl, arylalkyl, heterocyclyl, tetrazolyl, halogen, OH, CN, NO_2 and OR, where R is alkyl, NHR, where R is H and alkyl, COOR, where R is H, and alkyl, SO_3R, where R is H and alkyl, SO_2NHR, where R is H and alkyl.

7. The compound of claim 4, wherein the group alkyl is substituted straight or branched alkyl chains carrying 1 to 6 carbon atoms.

8. The compound of claim 5, wherein alkyl is methyl, ethyl, n-propyl, i-propyl, n-butyl, i-butyl or tert-butyl.

9. The compound of claim 4, wherein alkenyl is substituted straight or branched alkenyl chains carrying 2 to 6 carbon atoms.

10. The compound of claim 9, wherein the alkenyl is vinyl, 1-propenyl, 2-propenyl, i-propenyl, butenyl or its isomers.

11. The compound of claim 4, wherein alkynyl is substituted straight or branched alkynyl chains carrying 2 to 6 carbon atoms.

12. The compound of claim 11, wherein alkynyl group is ethynyl, propynyl or its isomers, or butynyl or its isomers.

13. The compound of claim 4, wherein suitable substituents of alkyl, alkenyl and alkynyl can be selected from one or more of amino, cyano, halogen, hydroxy, alkoxy, aryloxy, aryl, heterocyclyl, carboxy, nitro, alkyl sulfonyl, aryl sulfonyl, thio, alkyl thio, or aryl thio.

14. The compound of claim 4, wherein cycloalkyl is substituted cycloalkyl groups containing 3 to 6 carbon atoms.

15. The compound of claim 14, wherein the cycloalkyl is cyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl, cycloheptyl, or adamantyl.

16. The compound of claim 14, wherein the cycloalkyl is benz-fused to an aromatic cyclic group.

17. The compound of claim 13, wherein the aryl is ~~sub~~stituted phenyl or napthyl.

18. The compound of claim 4, wherein the group heterocyclic is optionally substituted with saturated, partially saturated, or aromatic cyclics, which contain one or more heteroatoms selected from nitrogen, oxygen or sulfur.

19. The compound of claim 18, which is benz-fused to a substituted aromatic cyclic or heterocyles.

20. The compound of claim 4, wherein the heterocyclic group is quinolinyl, pyridyl, indolyl, furyl, oxazolyl, thienyl, triazolyl, pyrazolyl, imidazolyl, benzothiazolyl, benzimidazolyl, piperzinyl, or benzothiazolyl.

21. The compound of claim 4, wherein the halogen group is chloro, bromo, fluoro, or iodo.

22. A compound having formula I, which is acidic and capable of forming pharmaceutically acceptable salts with inorganic and organic bases.

23. The compound of claim 22, wherein the base is sodium hydroxide, potassium hydroxide, calcium hydroxide, barium hydroxide, magnesium hydroxide, or N-ethyl piperidine.

24. The compound having formula I, which forms pharmaceutically acceptable salt with inorganic and organic acids.

25. The compound of claim 24, wherein the acid is hydrochloric acid, sulfuric acid, nitric acid, phosphoric acid, acetic acid, tartaric acid, succinic acid, fumaric acid, maleic acid, malic acid, citric acid, or methane sulfonic acid.

26. The compound of claim 4, wherein X is C; R_1 and R_2 are CH_3 respectively; and R_3 is H; and R_4 is OH; and R_5 is COOH and R_6, R_7, R_8 and R_9 are each H.

27. The compound of claim 4, wherein R_1, R_2 and R_3 are H respectively; and R_4 is COOH, R_5 is Cl, and R_6, R_7, R_8 and R_9 each are H and X is C.

28. An antiviral pharmaceutical composition comprising an effective amount of a compound with formula I, or a pharmaceutically acceptable salt, and a pharmaceutically acceptable carrier.

29. The pharmaceutical composition of claim 28 for treating human immunodeficiency virus (HIV) infection, further comprising effective amount of an Acquired Immunodeficiency Syndrome (AIDS) treatment agent selected from the group consisting of anti-HIV agents, anti-infective agents, and immunomodulators.

30. A method for inhibiting replication of human immunodeficiency virus in cells comprising contacting cells with an effective amount of a compound with formula I to inhibit the replication of the human immunodeficiency virus.

31. A method for treating mammals infected with the human immunodeficiency virus, comprising administering to said mammals an effective amount of a compound with formula I, or its pharmaceutically acceptable salts thereof.

32. A method for preventing manifestation of Acquired Immunodeficiency Syndrome (AIDS) in a subject comprising administering to the subject an amount of a compound with formula I effective to prevent said syndrome in the subject.

33. A method for screening compounds for inhibition of HIV infection using a monoclonal antibody which reacts with the fusion-active gp41 core structure and binds specifically to a trimer of a heterodimer formed by an N-peptide and a C-peptide, but not to the individual N-Peptide and C-peptide and a biological assay.

34. The method of claim 33, wherein the assay is fluorescence native polyacrylamide gel electrophoresis (FN-PAGE).

35. The method of claim 33, wherein the biological assay is a virus-cell or cell-cell fusion assay.

36. The compound resulting from the screening method of claim 33 to 35.

37. A composition comprising the compound of claim 36.

38. A pharmaceutical composition comprising an amount of the compound of claim 35 effective to inhibit HIV replication and a pharmaceutically acceptable carrier.